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Supplementary Info for RSC Advances revised article

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1 CALCULATIONS OF THE AMOUNT OF DOX ON GOLD NANOTRIANGLES IN MG OF DOX PER ML OF THE NANOPARTICULATE SOLUTION FOR BIOLOGICAL STUDIES.

Total volume of the solution of nanoparticles = 0.034 dm^3

Molar attenuation coefficient

Control solution - solution taken for the synthesis of AuNTs-PEG-DOX, having the same composition except the AuNTs. It allowes us to count the attenuation coefficient of this system and thus the concentration of DOX on AuNTs-PEG-DOX. Absorbance of the control = 0.5048, concentration of DOX is known and equal 4.78×10^{-5} M, l = 1 cm. From Lambert-Beer formula: $A = \epsilon l c$

$$\epsilon = \frac{A_{control}}{l \cdot C_{control}} = 10560.66946 \frac{dm^3}{cm \cdot mol}$$

Concentration of excess DOX in post-synthetic supernatant

Absorbance of the supernatant solution left after the synthesis of AuNTs-PEG-DOX = 0.4101 (absorbance of the supernatant collected after conjugation of DOX - absorbance of the excess of DOX). Knowing the molar attenuation coefficient, we were able to count the concentration of the excess DOX in the supernatant.

C of DOX in supernatant solution = $\frac{A}{\epsilon l} = 3.8835 \times 10^{-5}$ M

General concentration of DOX on AuNTs-PEG-DOX

The difference (ΔC) between the concentrations of DOX in the control and the concentration of excess DOX in the supernatant allowed us to calculate how much DOX was bound to AuNTs modified with PEG (Fig. 1.1).

$\Delta C = C_{DOX_{control}} - C_{DOX_{supernatant}} = 8.965 \times 10^{-6}$ M - C of DOX on AuNTs-PEG-DOX

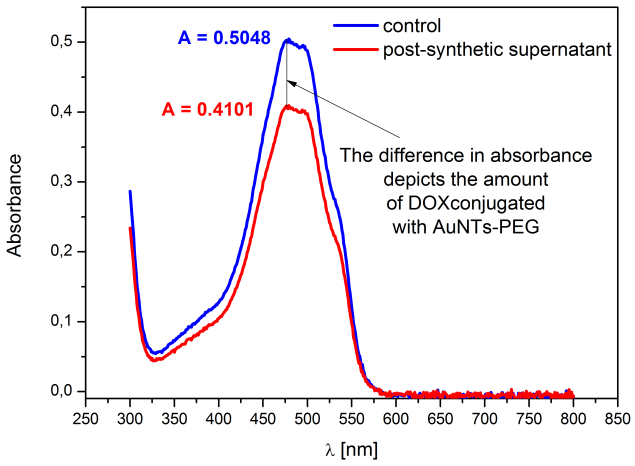

Figure 1.1: UV-Vis spectra allowing the calculations of the amount of DOX bount to AuNTs-PEG.

The amount of gold used in the synthesis of AuNTs

m of chloroauric acid taken for the synthesis of NTs = 17.605 mg

$M_{Au} = 197 \frac{g}{mol}$

$M_{HAuCl_4 * 4H_2O} = 411.84 \frac{g}{mol}$

Therefore, m of gold taken for the synthesis:

$m_{Au} = \frac{M_{Au}}{M_{HAuCl_4}} \cdot m_{HAuCl_4} = \frac{197}{411.84} \cdot 17.605 = 8.42$ mg

Concentration of DOX in mol DOX/mg Au of solution of AuNTs-PEG-DOX

$n_{DOX} = \Delta C \cdot 0.034 = 3.048 \times 10^{-7}$ mol

$m_{Au} = 8.42$ mg

C in mol DOX/ mg Au= $\frac{nDOX}{mAu} = \frac{3.048 \times 10^{-7}}{8.42} = 3.61995 \times 10^{-8} \frac{mol_{DOX}}{mg_{Au}}$

Concentration of DOX in mol DOX/mL of solution of AuNTs-PEG-DOX dissolved in DMSO
The post synthetic centrifuged pellet of AuNTs-PEG-DOX was dissolved in small amount of DMSO. 1 mL of this solution was left to dry (to evaporate the solvent) and the dried mass was weighted. The concentration of the NTs in mg/mL after drying was equal 5 mg/mL.
Using this information we were able to count the concentration of DOX given in moles per mL of nanotriangles solution (dissolved in DMSO).

C (in mol DOX/mg Au) $\cdot$ 5 mg/mL = 3.61995×10^{-8} mol DOX/ mg Au $\cdot$ 5 mg/mL = 1.81×10^{-7} mol DOX/mL of solution of AuNTs-PEG-DOX

Concentration of DOX in mg DOX/mL of solution of AuNTs-PEG-DOX dissolved in DMSO
Next, knowing the molar mass of DOX, that is equal 579.98 g/mol, we were able to calculate the concentration of DOX in mg of DOX per mL of nanoparticulate solution.

1.81×10^{-7} mol DOX/mL $\cdot$ 579.98 g/mol = 1.05×10^{-4} g DOX/ mL = 10.5 mg DOX/ mL - concentration of DOX on gold nanotriangles (in the solution used in MTT, which will be later diluted).